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# Inverted Pairing and Excitation Induced by Quadrupole-Quadrupole Interaction

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## Abstract

In this paper, it is shown for a single- $j$  shell that the intrinsic excitations induced by the quadrupole-quadrupole interaction can be viewed as that due to the inverted surface-delta interaction whose multipole-pairing component with the largest spin is the dominant term and is attractive. This allows us to trace the origin of the recently introduced optimum pair description of rotation and leads naturally to analytical expressions for the rotational energies for the various bands in a single  $j$ -shell with the quadrupole-quadrupole interaction

One of the central aims of nuclear structure physics is to understand how strong collectivity is manifested in the spherical shell model. Since straightforward application of the shell model is not possible for strongly deformed systems, a great deal of effort in the past forty years was devoted to the development of suitable truncation schemes to confront this problem <sup>1, 2</sup>.

It is well known now that under a strong monopole pairing interaction plus a weak quadrupole-quadrupole (QQ) interaction, monopole and quadrupole pairs appear to be a good truncation scheme. However, when the QQ interaction becomes dominant, it appears that higher multipoles, especially the hexadecapole pairs, must be added <sup>3</sup>.

On the other hand, it has been recently been shown that the eigenstates of the pure QQ interaction in a single- $j$  shell can be well described in terms of a collection of optimum pairs, using a novel approach which was proposed to describe nuclear states within a spherical shell model with an optimum pair basis<sup>4</sup>. This paper aims to trace the origin of such a description of rotation in a single- $j$  shell with the strong QQ interaction. The physics behind this approach can be easily understood as follows. The major part of the QQ interaction in the single  $j$  shell can be expressed as a constant plus an  $L^2$  term. The remaining parts can be simulated by an inverted Surface-Delta-Interaction (SDI), which will favor higher spin pairs. The constant plus the  $L^2$  terms can be exactly diagonalized. This will give the rotational spectrum. The remaining part (i.e. the inverted SDI) can be approximately diagonalized by using first the standard many-body Tamm-Dancoff approximation, followed by the optimum pair approach. A by-product of this study is the derivation of analytical expressions for the rotational energies for various bands, for a system of any number of pairs moving in a single  $j$  shell, although the number dependence is not understood at this point. In hindsight, this approach is possible because the intrinsic excitations induced by the QQ-interaction comes essentially from the inverted SDI.

We shall illustrate our method via a simple solvable model: like-particles moving in a single- $j$  shell. This example is chosen because the QQ-interaction can simulate the rotational excitation structure<sup>2</sup>. For a system of  $n/2$  or  $N$  pairs of nucleons in single- $j$  shell, the most

general Hamiltonian is

$$\mathbf{H} = \epsilon_j \sqrt{2j+1} (\mathbf{a}_j^\dagger \times \tilde{\mathbf{a}}_j)^0 + \sum_{\Lambda} \sqrt{2\Lambda+1} C_{\Lambda} (\mathbf{A}_{\Lambda}^\dagger \times \tilde{\mathbf{A}}_{\Lambda})^0 \quad (1)$$

with

$$\mathbf{A}_{\Lambda}^\dagger = \frac{1}{\sqrt{2}} (\mathbf{a}_j^\dagger \times \mathbf{a}_j^\dagger)^\Lambda \quad (2)$$

and

$$C_{\Lambda} = \langle jj\Lambda \parallel \mathbf{V} \parallel jj\Lambda \rangle \quad (3)$$

where  $\mathbf{a}_j^\dagger$  ( $\tilde{\mathbf{a}}_j$ ) are the creation (annihilation) operators with energy  $\epsilon_j$ .

Using the equation-of-motion technique<sup>5</sup>, we shall employ the many-pair creation operator as the excitation operator and the Tamm-Dancoff vacuum as the "true" vacuum. To portray a collection of multipole pair excitations, the excitation operator is expressed as a simple tensor product:

$$\Omega^\dagger = \mathbf{A}_1^\dagger \mathbf{A}_2^\dagger \dots \mathbf{A}_N^\dagger \quad (4)$$

where  $\mathbf{A}_i^\dagger$  stands for  $\mathbf{A}_{L_i}^\dagger$ , the tensor of rank  $L_i$ .

Following the standard process of linearization, the corresponding equation-of-motion becomes

$$[\mathbf{H}, \Omega^\dagger] = E_T \Omega^\dagger \quad (5)$$

and the TDA energies are

$$E_T = \sum_{\Lambda} N_{\Lambda} C_{\Lambda} \quad (6)$$

Here  $N_{\Lambda}$  is the number of such pairs with angular momentum  $\Lambda$ .

It is known that the TDA is most valid when  $j$  is large and for interactions such as surface delta where the strengths of the multipole pairing components decrease monotonically. It is unsuitable for the identity interaction and the QQ force. For example, one can easily show

that the TDA ground state energy for four particles in  $j = 21/2$  orbit is only a third (a fifth) of the exact value for the identity (QQ) interaction. However, as will be shown later, the inadequacy of the TDA for these interactions can be salvaged by the introduction of an auxiliary Hamiltonian to the QQ force which will render it as an "inverted" SDI interaction, one in which the strengths of the new multipole pairing components increase rather than decrease monotonically. It will restore the validity of the TDA. To this end, we shall introduce the following auxiliary Hamiltonian as

$$H' = H_{QQ} - \alpha \sum_{i < j} I_{ij} - \gamma \mathbf{L}^2 \quad (7)$$

where  $\mathbf{L}$  is the angular momentum operator and  $I_{ij}$  stands for the identity interaction and  $\mathbf{L}$  and  $I_{ij}$  are so chosen for their simplicity in representing an exact symmetry of the system. In fact, the auxiliary Hamiltonian of Eq.(7) has the same form as the original one given by Eq.(1) if the interaction matrix element, or multipole-pairing strength, are redefined as

$$C'_\Lambda = C_\Lambda - \alpha - \gamma[\Lambda(\Lambda + 1) - 2j(j + 1)] \quad (8)$$

where the parameters  $\alpha$  and  $\gamma$  in (8) are determined by expressing this new Hamiltonian as an inverted SDI with the following choice

$$\begin{aligned} \alpha &= \frac{10 - j(j + 1)}{7} \mathbf{C}_2 + \frac{j(j + 1) - 3}{7} \mathbf{C}_4 \\ \gamma &= \frac{1}{14} (\mathbf{C}_4 - \mathbf{C}_2) \end{aligned} \quad (9)$$

Explicitly, they are

$$\alpha = \frac{20(j - 2)(j + 3)(2j - 3)(2j + 5)}{j(j + 1)(2j - 1)(2j + 1)(2j + 3)} \quad (10)$$

$$\gamma = \frac{15[4j(j + 1) - 27]}{j(j + 1)(2j - 1)(2j + 1)(2j + 3)} \quad (11)$$

Using the above parameters, one can show that the multipole pairing strength  $C'_\Lambda$  are

$$C'_\Lambda = -\frac{15(\Lambda - 2)(\Lambda + 3)(\Lambda - 4)(\Lambda + 5)}{j(j + 1)(2j - 1)(2j + 1)(2j + 3)} \quad (12)$$

The invertness can also explicitly be seen numerically. For  $j=21/2$ , the values of multipole-pairing strengths are

$$[-0.001, 0, 0, -0.0093, -0.04, -0.11, -0.24, -0.46, -0.79, -1.27, -1.95]$$

for  $\Lambda = 0, \Lambda = 2, \Lambda = 4, \dots, \Lambda = 20$ .

Applying TDA to the inverted SDI, we can obtain the following energy expression:

$$E = \sum_{\Lambda} N_{\Lambda} C'_{\Lambda} + \frac{n(n-1)}{2} \alpha + \gamma [L(L+1) - nj(j+1)] \quad (13)$$

Here the TDA energies,  $\sum_{\Lambda} N_{\Lambda} C'_{\Lambda}$  are degenerate for all  $L$  values and thus serve as the intrinsic states from which the various rotational bands are built. The intrinsic excitations are the pairs with the energy  $C'_{\Lambda}$ . The expression (13) with the numerical values of (12) clearly indicate that the pairs with the lowest energy does indeed have the highest spin, and hence the system's ground state must be due to the contribution of  $N$  pairs of nucleons, each coupled to the highest spin ( $\Lambda = 2j - 1$ ). This is of course precisely the behavior demonstrated in a pair shell model calculation with the optimal pair approximation<sup>3</sup>. For the two pair case, the ground band is labeled as  $(2j - 1; 2j - 1)$  since it is formed by two  $2j - 1$  pairs and the spin sequence of the band is  $0, 2, 4, 6, \dots$ , while the first excited band is a  $(2j-3; 2j-1)$ -band (one  $2j - 3$  pair and one  $2j - 1$  pair) with the  $\gamma$ -band spin sequence of  $2, 3, 4, 5, \dots$ . Finally, the  $\beta$ -band comes from coupling two  $2j - 3$ -pairs.

In Table I, results for a system of four particles in a  $j = 21/2$  orbit are presented. In particular, the above approximation is compared with the exact shell model calculations. In this approximation, the values of  $C'_{\Lambda}$  are given by (12), referred to as Approx. I. This distinguishes it from the other choices of  $C'_{\Lambda}$  mentioned below. In view of the simplicity of the model, the agreement is quite good.

It is interesting to note that the above choice of  $C'_{\Lambda}$  is close to that of fixing  $\alpha$  and  $\gamma$  in (8) which result in cancelling the  $a + b\Lambda(\Lambda + 1)$  terms in the  $C_{\Lambda}$  for QQ interaction. This latter is given as  $10W(jjjj; 2\Lambda)$  and can be expanded in  $\Lambda(\Lambda + 1)$ :

$$C_{\Lambda} = a + b\Lambda(\Lambda + 1) + c\Lambda^2(\Lambda + 1)^2 \quad (14)$$

where

$$a = -\frac{10}{2j+1}$$

$$b = \frac{15(4j(j+1)-1)}{j(j+1)(2j-1)(2j+1)(2j+3)}$$

$$c = -\frac{15}{j(j+1)(2j-1)(2j+1)(2j+3)}$$

The  $\alpha$  and  $\gamma$  thus determined are

$$\alpha = \frac{80j(j+1)}{(2j-1)(2j+1)(2j+3)} \quad (15)$$

$$\gamma = \frac{15(4j(j+1)-1)}{j(j+1)(2j-1)(2j+1)(2j+3)} \quad (16)$$

and the new multipole pairing strengths are

$$C'_\Lambda = -\frac{15\Lambda^2(\Lambda+1)^2}{j(j+1)(2j-1)(2j+1)(2j+3)} \quad (17)$$

which are numerically close to that given by (12) (See Table II).

The above results imply that one can decompose the multipole pairing strengths in the QQ-interaction into the collective part  $a+b\Lambda(\Lambda+1)$  and the intrinsic part  $c\Lambda^2(\Lambda+1)^2$ . The latter contributes to the intrinsic energies of TDA. The approximation led by this choice of  $C'_\Lambda$  is given as Approx.II in Table I.

Besides the above choices of  $\alpha$  and  $\gamma$  which led to the inverted SDI-like interactions, an additional one is added in which the parameters are fixed so that  $C'_\Lambda$  is as close to an inverted SDI as possible. A strict inverted SDI is defined as

$$C_\Lambda^{IV} = \frac{2}{2j+1} C_{2j-1-\Lambda}^{SDI} \quad (18)$$

and the  $\chi^2$ -fit treatment would lead to the following expressions for  $\alpha$  and  $\gamma$ :

$$\gamma = \frac{\langle (C_\Lambda - C_\Lambda^{IV})\Lambda(\Lambda+1) \rangle - \langle (C_\Lambda - C_\Lambda^{IV}) \rangle \langle \Lambda(\Lambda+1) \rangle}{\langle \Lambda^2(\Lambda+1)^2 \rangle - \langle \Lambda(\Lambda+1) \rangle^2} \quad (19)$$

$$\alpha = \langle (C_\Lambda - C_\Lambda^{IV}) \rangle - \gamma [\langle \Lambda(\Lambda + 1) \rangle - 2j(j + 1)] \quad (20)$$

where  $\langle \dots \rangle$  represents the average taken as

$$\frac{\sum_{\Lambda=0}^{\frac{2j-1}{2}} (2\Lambda + 1)(\dots)}{\sum (2\Lambda + 1)}$$

When these are applied to the QQ force, the resulting analytical expressions are complicated and not physically transparent. If one chooses the following simple expressions (which will fit (19) and (20) well),

$$\alpha = \frac{80(j-3)(j+4)(j-5)(j+6)}{j(j+1)(2j-1)(2j+1)(2j+3)} \quad (21)$$

$$\gamma = \frac{60(j-5)(j+6)}{j(j+1)(2j-1)(2j+1)(2j+3)} \quad (22)$$

one can obtain the results as presented in Tables I and II (denoted as Inverted SDI).

The comparisons we presented in Table I with the various choices of  $C'_\Lambda$  suggest that the TDA with the inverted-SDI is an excellent caricature of the exact shell model calculations for the single- $j$  case. Consequently, the intrinsic excitations induced by the QQ-interaction are described according to our simple model (13) as elementary with energies  $C'_\Lambda$ , from which all the rotational bands are built upon, which are the multipole-pairing strengths in an inverted SDI. We therefore conclude from (8) that the "intrinsic" part of the QQ force is equivalent to an inverted SDI. With this view point, one can understand the origin of the optimum pair description of rotation. In physical terms, the short range delta force will favor the S-pairs, the QQ force favors high spins pairs whose field is generated by an inverted SDI.

The present model given by Eq. (13) has two shortcomings. The first is the moment of inertias are identical for all bands and the second is that the parameter  $\alpha$  is independent of the elementary excitations. Using a more rigorous treatment, (shown next) for the TDA for arbitrary interactions, the above results can be improved. In this treatment, which is akin to the generalized pair field method (GPFM)<sup>4</sup>, the results for the QQ interaction are nearly exact and more importantly, the moment of inertia can vary from band to band.

We thus begin by considering the commutator of the auxiliary Hamiltonian

$$\mathbf{H}' = \mathbf{H} - \omega \sum_{i < j} I_{ij} \quad (23)$$

and  $\Omega^\dagger$  in (4).  $\mathbf{H}'$  can formally be expanded as

$$[\mathbf{H}', \Omega^\dagger] = E'_T \Omega^\dagger + \sum_{1'2' \dots N'} \Phi(12 \dots N; 1'2' \dots N'; \omega) (\mathbf{A}_1^\dagger, \mathbf{A}_{2'}^\dagger, \dots, \mathbf{A}_{N'}^\dagger)^L \quad (24)$$

where  $\omega$  is chosen by a  $\chi^2$ -fit with only the first term surviving. Again, the TDA is made valid by the proper choice of the new Hamiltonian!

For a system of four particles moving in a single  $j$ -orbit, the  $\omega$ , after  $\chi^2$ -fitting, takes on the form

$$\omega = \frac{\sum_{L'_1 L'_2} (C_{L'_1} + C_{L'_2}) (2L'_1 + 1) (2L'_2 + 1) X^2(jjL_1; jjL_2; L'_1 L'_2 L)}{2 \sum_{L'_1 L'_2} (2L'_1 + 1) (2L'_2 + 1) X^2(jjL_1; jjL_2; L'_1 L'_2 L)} \quad (25)$$

where  $X$  is a 9 $j$ -symbol. Note that unlike  $\alpha$  in (9),  $\omega$  is not a constant depends on  $L_1 L_2 L$ . This means that for the various bands, it will have different contributions to the elementary excitations. In addition, since it depends on  $L$ ,  $\omega$  can cover more than the term  $\alpha + \gamma(\Lambda(\Lambda + 1) - 2j(j + 1))$  in (8) which is only limited to the rigid rotor case.

For any general interaction  $C_\Lambda$ , the  $\omega$  in (25) is usually computed numerically. However, for QQ, we are able to find analytical solutions for the two pair case.

Using  $C_\Lambda^{QQ} = 10W(jjjj; 2\Lambda)$  for QQ, one can derive the following expressions:

$$\omega^{QQ} = - \frac{10(2L_1 + 1)(2L_2 + 1)F_2 + (2L_1 + 1)(2L_2 + 1) \sum_k (-1)^k (2k + 1) C_k^{QQ} F_k}{1 + \delta_{L_1 L_2} - 2(2L_1 + 1)(2L_2 + 1) X(jjL_1; jjL_2; L_1 L_2 L)} \quad (26)$$

where  $F_k$  is given by

$$F_k = W(L_1 j L_1 j; jk) W(L_2 j L_2 j; jk) W(L_1 L_2 L_1 L_2; Lk) \\ + W(L_1 j L_2 j; jk)^2 W(L_1 L_2 L_2 L_1; Lk). \quad (27)$$

For the QQ-interaction,  $\omega^{QQ}$  turns out to be simple in which the largest spin pairs are preferred to be chosen as optimum pairs. One can numerically show that both the second term in the numerator and the denominator, and the second term of Eq.(27) are all shown to be negligible. Thus,



$$\omega^{QQ} = -\frac{10}{1 + \delta_{L_1 L_2}}(2L_1 + 1)(2L_2 + 1) \quad (28)$$

$$\times W(L_1 j L_1 j; j 2) W(L_2 j L_2 j; j 2) W(L_1 L_2 L_1 L_2; L 2)$$

This expression will reproduce well the exact values for the low-lying bands. The detail comparisons with the exact results are given in Fig. 1.

With this  $\omega$ , we can now cast the total energy into an analytical form:

$$E = E_o + \frac{\hbar^2}{2\mathfrak{I}} L(L+1) - \chi L^2(L+1)^2 \quad (29)$$

where  $E_o$  is the intrinsic energy given by

$$E_o = C_{L_1}^{QQ} + C_{L_2}^{QQ} - \chi \left[ \bar{L}_1^4 + \bar{L}_2^4 - \bar{L}_1^2 - \bar{L}_2^2 + \frac{2}{3} \bar{L}_1^2 \bar{L}_2^2 \right] \quad (30)$$

with the  $\chi$  in the form

$$\chi = \frac{15[3\bar{L}_1^2 - 4\bar{j}^2 - 3][3\bar{L}_2^2 - 4\bar{j}^2 - 3]}{j(j+1)(2j-1)(2j+1)(2j+3)(2L_1-1)(2L_2-1)(2L_1+3)(2L_2+3)} \quad (31)$$

and  $\bar{L}_i = \sqrt{L_i(L_i+1)}$ ,  $\bar{j} = \sqrt{j(j+1)}$ . The moments of inertia are found to be

$$\frac{\hbar^2}{2\mathfrak{I}} = \chi[2\bar{L}_1^2 + 2\bar{L}_2^2 - 1] \quad (32)$$

The term  $\chi L^2(L+1)^2$  which causes deviation from the rigid rotor expression is in fact negligible for the QQ-interaction.

Since the choice of  $\omega^{QQ}$  taken from a four-particle system is more accurate than those of  $\alpha$  and  $\gamma$  in (9), we now return to the rotational limit of the many particle system (13) and seek a better set of values them, extracted from Eq.(29). We thus set

$$C_{L_1}^{QQ} + C_{L_2}^{QQ} + 4\alpha - \gamma [L_1(L_1+1) + L_2(L_2+1)] = E_o \quad (33)$$

from which one can obtain  $\alpha$  and  $\gamma$ :

$$\alpha = \frac{\chi}{4} \left[ \bar{L}_1^4 + \bar{L}_2^4 + \frac{10}{3} \bar{L}_1^2 \bar{L}_2^2 \right]$$

$$\gamma = \frac{\hbar^2}{2\mathfrak{I}} = \chi [2\bar{L}_1^2 + 2\bar{L}_2^2 - 1] \quad (34)$$

Since these expressions are extracted from the nearly exact solutions of the four particle problem, their ability to reproduce the inverted SDI-like behavior, as given by Eq.(8), is a confirmation of the physics so far discussed. Together with the former ones, the results of the moments of inertia and the various band heads, calculated according to this choice of parameters, are presented in Table I (listed as 2-Pair Fit). The values of  $C'_\Lambda$  are listed in Table II. It is interesting to observe that these results are indeed close to the inverted SDI ones and the exact SM. Of course, it remains to be seen whether these expressions can be generalized to the system of an arbitrary number of pairs.

In conclusion, we have presented evidence in this paper that the excitations induced by the QQ-interaction is equivalent to the inverted surface-delta interaction whose multipole-pairing component is dominant and attractive for the largest multipole. This thus provide an understanding of the origin of the recently introduced optimum pair description of rotation. Finally, it should be emphasized that the present approach possesses a predictive power for the excited bands using a simple Tamm-Dancoff approximation.

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Table I

Inverted SDI vs EXACT SM

<i>Methods</i>	$C'_{20}$	$\alpha$	$\gamma$	$\gamma - E$	$\beta - E$
Approx.I	-1.95	0.84	$5.4 \times 10^{-3}$	0.68	1.36
Approx.II	-2.08	0.91	$5.6 \times 10^{-3}$	0.70	1.40
Inverted SDI	-1.53	0.62	$4.3 \times 10^{-3}$	0.59	1.18
2-Pair Fit	-1.49	0.59	$4.2 \times 10^{-3}$	0.62	1.12
Exact SM	-1.47	0.58	* $4.2 \times 10^{-3}$	0.62	1.12

\*\* Note: In Exact SM and the 2-Pair Fit, the moments of inertia vary as follows:

(a)  $\frac{\hbar^2}{2\mathfrak{I}} = 4.2 \times 10^{-3}$  for g-band

(b)  $\frac{\hbar^2}{2\mathfrak{I}} = 3.3 \times 10^{-3}$  for  $\gamma$ -band

(c)  $\frac{\hbar^2}{2\mathfrak{I}} = 2.5 \times 10^{-3}$  for  $\beta$ -band

Table II

The Values of  $C'_\Lambda$ 

$\Lambda$	I	II	III	IV
0	-0.001	-0	-0.042	-0.029
2	0	-4.E-4	-0.034	-0.020
4	0	-0.005	-0.019	-0.004
6	-0.009	-0.021	-0.019	-0.014
8	-0.040	-0.061	-0.004	-0.018
10	-0.110	-0.142	-0.003	-0.006
12	-0.239	-0.286	-0.110	-0.081
14	-0.456	-0.519	-0.267	-0.232
16	-0.786	-0.870	-0.532	-0.490
18	-1.273	-1.376	-0.939	-0.891
20	-1.948	-2.075	-1.529	-1.473

Note. Column labels I,II,III and IV represent the following:

I. Approximation I

II. Approximation II

III. Inverted SDI

IV. Two Pair Fit